Sebuthylazine 7286-69-3 | DTXSID7058171

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Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		75%)	Test (25%	Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.93	22.5	0.93	22.1	0.93	22.1		

Model Results

Predicted value: 295 °C

Global applicability domain: Outside

Local applicability domain index: 1.58e-01

Confidence level: 6.01e-01

Nearest Neighbors from the Training Set

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Desmetryn Measured: 345 Predicted: 341 Image not found

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Measured: 345
Predicted: 341

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2,4,6-Tricyano-1,3,5-triazine

Measured: 262 Predicted: 264

Image not found

Tetranitromethane Measured: 126 Predicted: 133 Image not found

3-Methyl-1-phenyl-1H-pyrazol-5-

amine

Measured: 333 Predicted: 334